

PySTEMM: Executable Concept Modeling for K-12 STEM Learning

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Abstract—Modeling should play a central role in K-12 STEM education, where it could make classes much more engaging. A model underlies every scientific theory, and models are central to all the STEM disciplines (Science, Technology, Engineering, Math). This paper describes executable concept modeling of STEM concepts using immutable objects and pure functions in Python. I present examples in math, physics, chemistry, and engineering, built using a proof-of-concept tool called PySTEMM. The approach applies to all STEM areas and supports learning with pictures, narrative, animation, and graph plots. Models can extend each other, simplifying getting started. The functional-programming style reduces incidental complexity and code debugging.

Index Terms—STEM education, STEM models, immutable objects, pure functions

1 INTRODUCTION

A *model* is a simplified representation of part of some world, focused on selected aspects. A model underlies every scientific theory, and models are central to all STEM areas — science, technology, engineering, and mathematics — helping us conceptualize, understand, explain, and predict phenomena objectively. Children form mental models and physical models during play to understand their world. Scientists use bio-engineered tissue as a model of human organs. Computational modeling is revolutionizing science and engineering, as recognized by the 2013 Nobel Prize in Chemistry going for computational modeling of biochemical systems.

Previous research [Whi93], [Orn08] has shown significant learning benefits from model-building and exploring in STEM education. Students should create, validate, refute, and use models to better understand deep connections across subject areas, rather than mechanically drilling through problems. In this paper I demonstrate that executable concept modeling, based on using immutable objects and pure functions in Python:

- applies across multiple STEM areas,
- supports different representations and learning modes,
- is feasible and approachable,
- encourages bottom-up exploration and assembly, and
- builds deep understanding of underlying concepts.

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1.1 Executable Concept Models

A *concept model* describes something by capturing relevant concepts, attributes, and rules. A *concept instance* is a specific individual of a *concept type* e.g. NO₂ is a concept instance of the general concept type Molecule. The concept type Molecule might define a *formula* attribute for any molecule instance to list how many atoms of each element it contains. The concept instance NO₂ has one Nitrogen and two Oxygen atoms. This is similar to the idea from object-oriented programming of an object that is an instance of a class.

Concepts and attributes are chosen to suit a purpose. A different model of Molecule might describe atoms, functional groups, bonds, sites at which other molecules can interact, site geometry, and forces that govern geometry and interactions.

An *executable concept model* is represented on a computer, so concept instances and concept types can be manipulated and checked by the machine, increasing confidence in the model.

1.2 PySTEMM Models

“Executable” typically entails programming language complexity, debugging headaches, and distractions from the actual concepts under study. Much of this complexity stems from *imperative programming*, where variables and object attributes are modified as the program executes its procedures.

Functional programming is a good alternative. It uses (a) *immutable objects*, whose attribute values do not get modified by program code; and (b) *pure functions*, producing a result that depends solely on inputs, without modifying any other attributes or variables.

PySTEMM, by using immutable objects and pure functions, and providing multiple model representations, reduces need-less complexity and debugging. It uses the *Python* programming language to define executable concept models that have three parts:

1. **Structure:** A concept type is defined by a Python *class* that describes attributes together with their types (which can reference other concept types). A concept instance is a Python *object* instantiated from that class, with values for its attributes.
2. **Functions:** The pure functions that represent additional properties or rules on concept instances are defined as Python *methods* on the class¹.

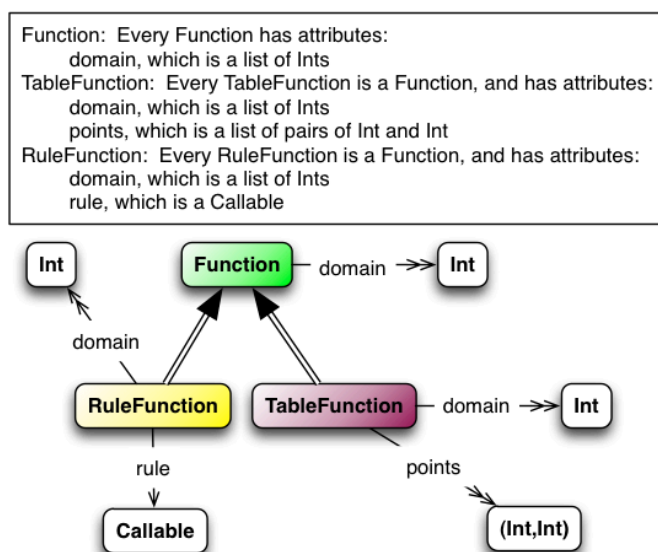


Fig. 1: Three Function concept types.

3. Visualization: The visualization of concept types and instances are defined with Python *dictionaries* of visual properties, used as *templates*.

PySTEMM models focus on defining *what terms and concepts mean*, rather than step-by-step instructions about *how to compute*. PySTEMM functions manipulate not just numbers, but molecules, rigid bodies, planets, visualizations, and even concept types and functions.

In the rest of this paper I present example models from math, chemistry, physics, and engineering, introduce key aspects of PySTEMM, and show Python model source code as well as multiple model representations generated by PySTEMM. The last section describes the implementation of PySTEMM.

2 MATHEMATICS

We begin with models of math functions, because math forms the basis of all other models. Next we move on to *high-order* functions i.e. functions that accept functions as inputs, or whose results are functions. Since our focus in this section is modeling math concepts, we will model math functions as objects. In subsequent sections on physics, chemistry, etc., we will directly use normal Python code for math computations.

2.1 Basic Numeric Functions

The Python model of *concept types* for basic functions is:

```
1 # file: function_types.py
2
3 class Function(Concept):
4     domain = Property(List(Int))
5     def eval(self, x): pass
6     class_template = {K.gradient_color: 'Green'}
7
8 class RuleFunction(Function):
9     rule = Callable
10    domain = List(Int)
```

1. Since we use methods on a class for functions, in " $a.f(x)$ " the inputs to f include argument x , and the object a on which the method is invoked.

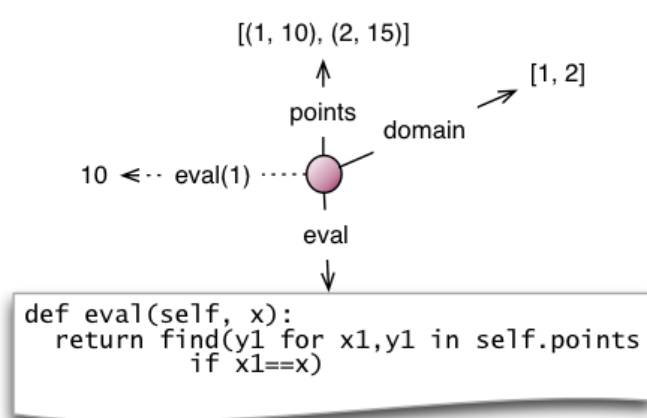


Fig. 2: TableFunction concept instance.

```
11
12 def eval(self, x):
13     return self.rule(x)
14
15 class_template = {K.gradient_color: 'Yellow'}
16
17 class TableFunction(Function):
18     points = List(Tuple(Int, Int))
19     domain = Property(List(Int))
20
21 def _get_domain(self):
22     return [x for x, y in self.points]
23
24 def eval(self, x):
25     return find(y1 for x1,y1 in self.points
26                if x1==x)
27
28 class_template = {K.gradient_color: 'Maroon'}
29 instance_template = {K.name: 'Circle'}
```

The concept type Function is defined as a class (line 3), with an attribute domain which is a list of integers (line 4). "Property" allows domain to be represented differently for different subclasses of Function. Function evaluation is modeled by method eval (line 5) whose specifics are deferred to subclasses. The visualization of functions is defined by class_template (line 6).

We define two subclasses of Function, each with different representations. RuleFunctions (line 8-15) are defined by an attribute rule that is a Python *callable* expression, an explicit domain, and eval that simply invokes rule. TableFunctions (line 17-29) are defined by a list of (x, y) pairs in an attribute points, a domain computed from points by _get_domain, and eval that finds the matching pair in points. The class_template (lines 15, 28) is a dictionary of visualization properties for the concept type, and instance_template (line 29) is for visualizing instances. PySTEMM generates the visual and English narrative in Figure 1 for these concept types.

Below, we *extend* this model with a TableFunction instance tf with its list of points (line 4), and customize what the model should visualize:

```
1 # file function_instances.py
2 from function_types.py import *
3
4 tf = TableFunction(points=[(1, 10), (2, 15)])
5
```

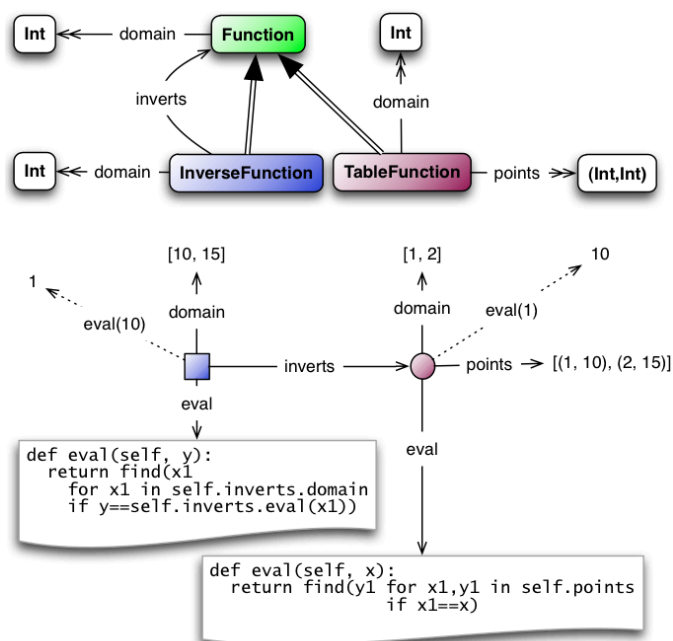


Fig. 3: *InverseFunction* type and instance.

```

6 M = Model()
7 M.addInstances(tf)
8 M.showMethod(tf, 'eval')
9 M.showEval(tf, 'eval', [1])

```

PySTEMM generates the visualization in Figure 2. The domain of *tf* was calculated from its points, its value at $x=1$ is 10, and the code for *eval()* is shown in the context of the instance. Since *eval* is a *pure function*, *tf.eval(1)* depends solely on the input 1 and the definition of *tf* itself, so it is easy to understand the source code: it returns the y_1 from the x_1, y_1 pair that matches the input x .

Note that *tf* is drawn as a circle of the same color as the *TableFunction* class: the *instance_template* for *TableFunction* is merged with the *class_template* before being applied to *tf*.

2.2 Inverse Functions

An *InverseFunction* inverts another: $g = f^{-1}(x)$. The model below extends the *function_instances* model with a class and an instance. On line 5, the *InverseFunction(...)* constructor is a *high-order function* corresponding to the f^{-1} operator, since it receives a function *tf* to invert, and produces the new inverted function *inv*.

```

1 from function_instances import *
2
3 class InverseFunction(Concept): ...
4
5 inv = InverseFunction(inverts=tf)
6
7 M.addClasses(InverseFunction)
8 M.addInstances(inv)
9 M.showEval(inv, 'eval', [15])

```

The instance visualization generated by PySTEMM in Figure 3 shows the inverse function as a blue square, its *eval()* effectively flips the (x, y) pairs of the function it inverts,

and its domain is computed as the set of y values of the function it inverts.

2.3 Graph Transforms and High-Order Functions

A graph transformation as taught in middle school — translation, scaling, rotation — is modeled as a function that operates on a source function, producing the transformed function. In Figure 4, PySTEMM generates a graph plot of the original function, a shifted version, and a “bumped” version of the shifted function. The instances are defined as:

```

Bump(source =
      ShiftX(source = RuleFunc(rule=square),
              by=3),
      start=0, end=5, val=100)

```

Similarly, the *limit* of a function is a high-order function: it operates on another function and a target point, and evaluates to a single numeric value. Calculus operators, such as *differentiation* and *integration*, can be modeled as high-order functions as well: they operate on a function and produce a new function.

3 CHEMISTRY: REACTION

```

1 class Element(Concept):
2     name = String
3
4 class Molecule(Concept):
5     formula = List(Tuple(Element, Int))
6     instance_template = {
7         K.text: lambda m: computed_label(m)
8     }
9 class Reaction(Concept):
10     products = List(Tuple(Int, Molecule))
11     reactants = List(Tuple(Int, Molecule))

```

An *Element* is modeled as just a name, since we ignore electron and nuclear structure. A *Molecule* has an attribute *formula* with a list of pairs of element with a number indicating the number of atoms of that element. A *Reaction* has *reactants* and *products*, each some quantity of a certain molecule. This Python model is visualized by PySTEMM in Figure 5.

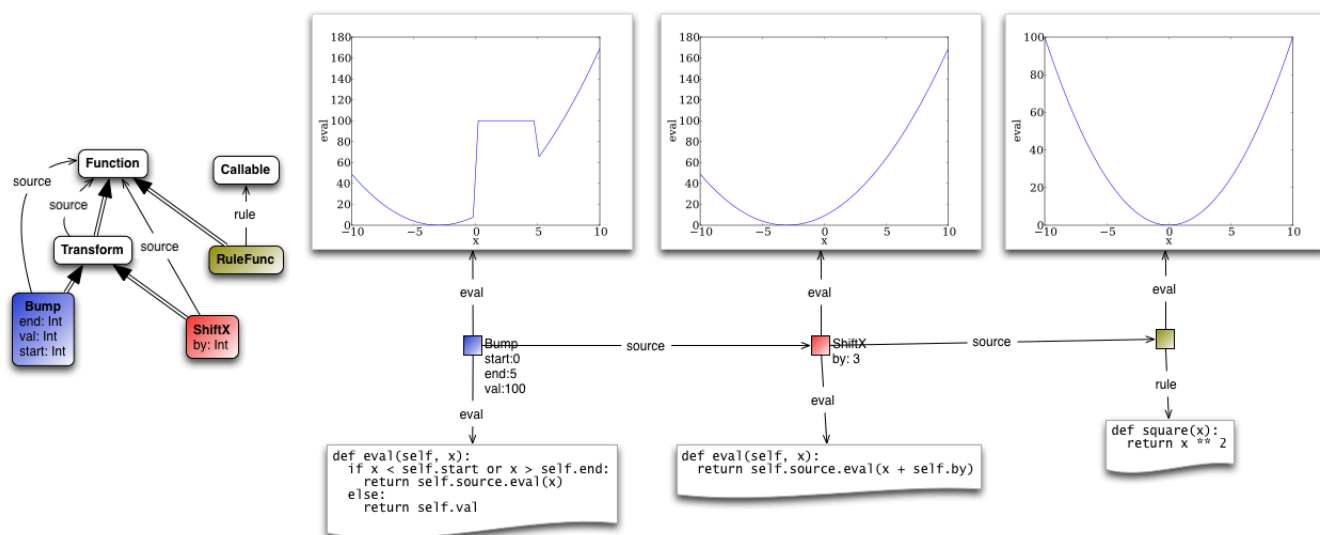
Note that convenient Python constructs, like *lists of tuples*, are visualized in a similarly convenient manner. Also, the *instance_template* for molecule (lines 6-7), specifying the visualization properties for a molecule instance, contains a *function* which takes a molecule instance and computes its label. Visualization templates are parameterized by the objects they will be applied to.

Figure 6 shows an instance of a reaction, showing reaction structure and computed labels for reactions and molecules, while hiding the formula structure within molecules.

3.1 Reaction Balancing

Our next model computes reaction balancing for reactions. An unbalanced reaction has lists *ins* and *outs* of molecules without coefficients. Figure 7 shows how PySTEMM visualizes a reaction with the balance computation, coefficients, and intermediate values, as explained below.

We formulate reaction-balancing as an *integer-linear programming* problem [Sen06], which we solve for molecule

Fig. 4: Function Transforms: A Bump of a Shift of x^2 .

Reaction: Every Reaction has attributes:
 reactants, which is a list of pairs of Int and Molecule
 products, which is a list of pairs of Int and Molecule
 Molecule: Every Molecule has attributes:
 formula, which is a list of pairs of Element and Int
 Element: Every Element has attributes:
 name, which is a String

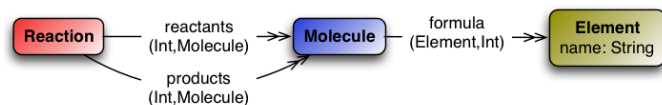


Fig. 5: Reaction concept type.

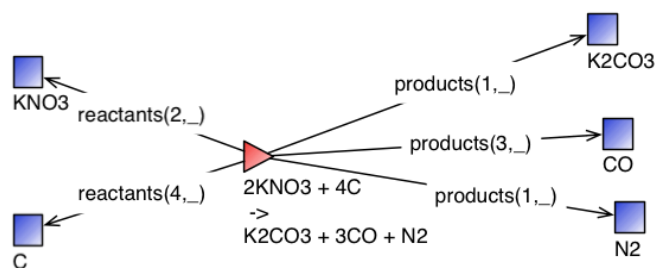


Fig. 6: An instance of Reaction.

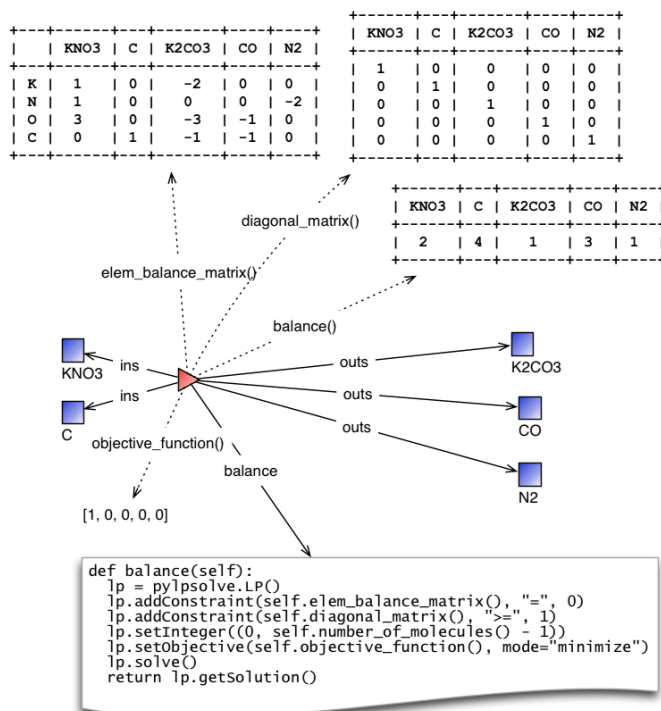


Fig. 7: Reaction balance matrix and solved coefficients.

coefficients. The formula of the molecules constrain the coefficients, since atoms of every element must balance. The function `elem_balance_matrix` computes a matrix of *molecule* vs. *element*, with the number of atoms of each element in each molecule, with + for ins and - for outs. This matrix multiplied by the vector of coefficients must result in all 0. All coefficients have to be positive integers (`diagonal_matrix`), and the `objective_function` seeks the smallest coefficients satisfying these constraints.

Once we have balanced reactions, we can add attributes and functions to model reaction stoichiometry and thermodynamics. For example:

```
class Element (Concept):
```

```
    name = String
    atomic_mass = Float

class Molecule (Concept):
    formula = List (Tuple (Element, Int))
    molar_mass = Property (Float)
    def _get_molar_mass (self):
        return sum([n * el.atomic_mass
                     for el, n in self.formula])

Fe = Element (name='Fe', atomic_mass=56)
Cl = Element (name='Cl', atomic_mass=35.5)
FeCl2 = Molecule (formula=[(Fe,1), (Cl,2)])
```

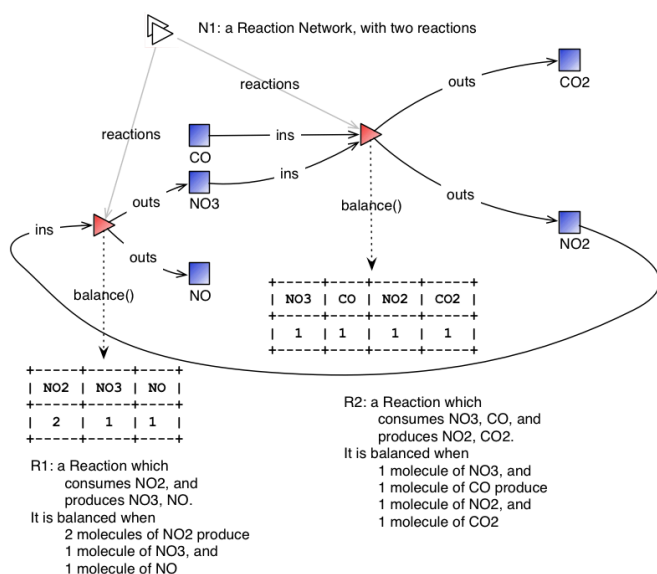



Fig. 8: A reaction Network with two reactions.

```
FeCl2.molar_mass # = 127
```

3.2 Reaction Network

```
class Network(Concept):
    reactions = List(Reaction)

R1 = Reaction(reactants=[(2, NO2)],
               products=[(1, NO3), (1, NO)])

R2 = Reaction(reactants=[(1, NO3), (1, CO)],
               products=[(1, NO2), (1, CO2)])

Net = Network(reactions=[R1, R2])
```

A Network of coupled chemical reactions has a list of reactions. Given this Python model, and a narrative template for Reaction, PySTEMM generates Figure 8, including the *instance-level* English narrative. Just as there are element balance constraints on an individual reaction, we could model network-level constraints on the reaction rates and concentrations of chemical species, but have not shown this here.

3.3 Layered Models

The reaction examples illustrate an important advantage of PySTEMM modeling; instead of directly modeling the mathematics of reaction, we focus on the structure of the concept instances; in this case, what constitutes a molecule, or a reaction?

From this model, we compute the math model. The math version of a molecule is a single column with the number of atoms of each element type in that molecule. The math for a reaction collects this column from each molecule and combines them into an `element_balance_matrix`. Pure functions thus easily traverse the concept instances to build corresponding math models such as matrices of numbers.

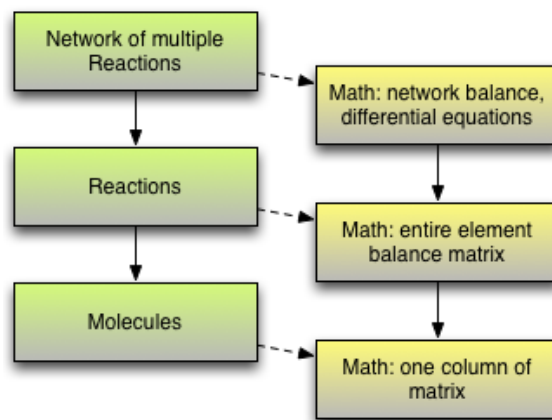


Fig. 9: Layered concept models and generated math.

4 PHYSICS

Below is a model of the motion of a ball under constant force. The ball has vector-valued attributes for initial position, velocity, and forces (lines 2,3). The functions acceleration, velocity, and position are pure functions of time and use numerical integration. We visualize ball `b` via `showGraph` and `animate` (lines 18-19). Like all visualizations, the animation is specified by a *template* (line 21): a dictionary of visual properties, except that these properties can be *functions* of the *object* being animated, and the *time* at which its attributes values are computed.

```
class Ball(Concept):
    mass, p0, v0 = Float, Instance(vector), ...
    forces = List(vector)
    def net_force(self):
        return v_sum(self.forces)
    def acceleration(self, time):
        return self.net_force() / self.mass
    def velocity(self, time):
        return self.v0 + v_integrate(self.acceleration, time)
    def position(self, time):
        return self.p0 + v_integrate(self.velocity, time)
    def p_x(self, time): ...
    def p_y(self, time): ...

b = Ball(p0=..., v0=..., mass=..., forces=...)
m = Model(b)
m.showGraph(b, ('a_y', 'v_y', 'p_y'), (0,10))
m.animate(b,
          (0,10),
          [{K.new: K.shape,
            K.origin: lambda b,t: [b.p_x(t), b.p_y(t)]},
           {K.new: K.line, point_list=lambda b,t: ...},
           {K.new: K.line, point_list=lambda b,t: ...}])
```

PySTEMM generates graphs of the time-varying functions, and a 2-D animation of the position and velocity vectors of the ball over time (Figure 10).

5 ENGINEERING

In Summer 2012 I attended the OEX program at MIT, where we designed and built a marine remote-operated vehicle (ROV) with sensors to monitor water conditions. I later used PySTEMM to recreate models of the ROV, and generate engineering attributes and 3-D visualizations like Figure 11.

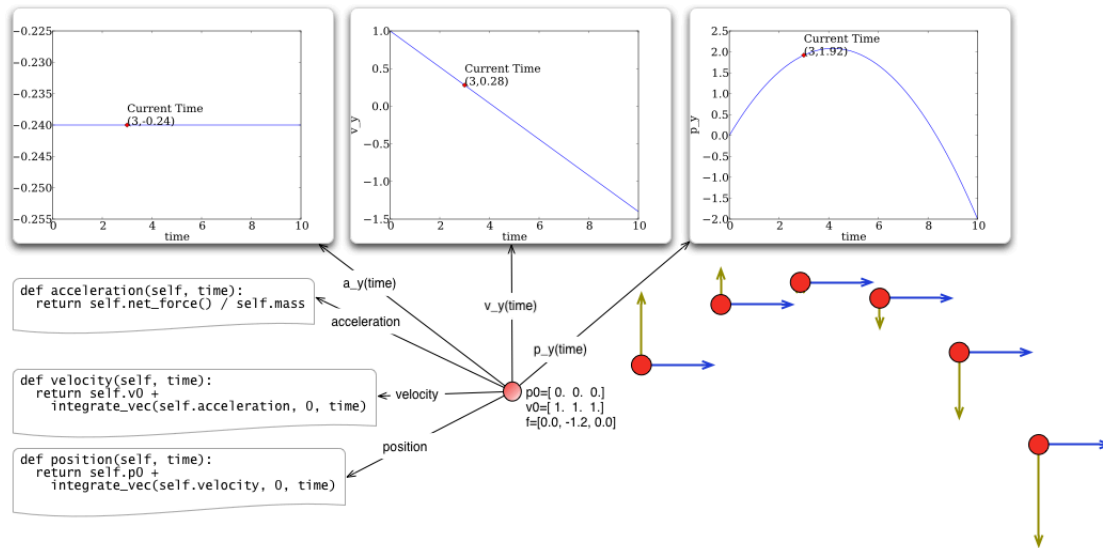


Fig. 10: Ball in motion: functions of time as code, graphs, animation

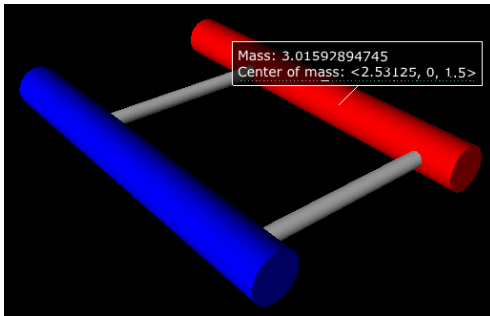


Fig. 11: ROV made of PVC Pipes.

The ROV is built from `PVC Pipes` in a functional style. To create several `PVC Pipes` positioned and sized relative to each other, the model uses pure functions like `shift` and `rotate` that take a `PVC Pipe` and some geometry, and produce a transformed `PVC Pipe`. This makes it simple to define parametric models and rapidly try different ROV structures. The model shown excludes motors, micro-controller, and computed drag, net force, and torque.

```
class PVCPipe(Concept):
    length, radius, density = Float, Float, Float
    def shift(self, v):
        return PVCPipe(self.p0 + v, self.r, self.axis)
    def rotate(self, a):
        return PVCPipe(self.p0, self.r, self.axis + a)

class ROV(Concept):
    body = List(PVCPipe)
    def mass(self): ...
    def center_of_mass(self): ...
    def moment_of_inertia(self): ...
```

```
p1 = PVCPipe(...)
p2 = p1.shift((0,0,3), ...)
c1, c2 = p1.rotate((0,0,90))...
rov = ROV(body=p1, p2, c1, c2)
```

6 IMPLEMENTATION

6.1 Architecture

The overall architecture of PySTEMM, illustrated in Figure 12, has two main parts: *Tool* and *Model Library*. The *tool* manipulates *models*, traversing them at the type and instance level and generating visualizations. The *model library* includes the models presented in this paper and any additional models any PySTEMM user would create. The *tool* is implemented with 3 classes:

- **Concept**: a superclass that triggers special handling of the concept type to process attribute-type definitions.
- **Model**: a collection of concepts classes and concept instances, configured with some visualization.
- **View**: an interface to a drawing application scripted via AppleScript.

Figure 12 explains the architecture in more detail, and lists external modules that were used for specific purposes. PySTEMM uses the Enthought `traits` module [Tra14] to define attribute types for a concept. Traits provides a class `HasTraits` with a custom meta-class, and pre-defined traits such as `List`, `Tuple`, `String`, and `Int`. The `Concept` class derives from `HasTraits`, which triggers traits to capture concept attribute type definitions and generate constructor and attribute logic for checked attribute assignment.

We gain several benefits by building models with immutable objects and pure functions:

- The *user models* can be manipulated by the *tool* more easily to provide tool capabilities like animation and graph-plotting, based on evaluating pure functions at different points in time.
- The values of computed attributes and other intermediate values can be visualized as easily and unambiguously as any stored attributes.
- Debugging becomes much less of an issue since values do not change while executing a model, and the definitions parallel the math taught in school science.

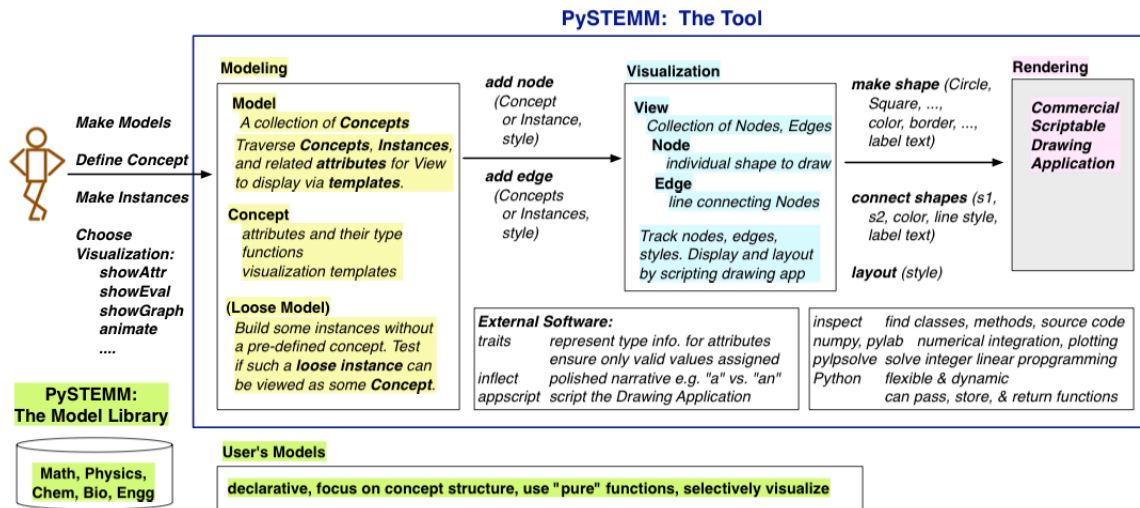


Fig. 12: Architecture of PySTEMM.

The source code for PySTEMM is available at <https://github.com/kdz/pystemm>.

6.2 Python

Python provides many advantages to this project:

- adequate support for high-order functions and functional programming;
- lightweight and flexible syntax, with convenient modeling constructs like lists, tuples, and dictionaries;
- good facilities to manipulate classes, methods, and source code;
- vast ecosystem of open-source libraries, including excellent ones for scientific computing.

6.3 Templates

All visualization is defined by *templates* containing visual property values, or functions to compute those values:

```
Concept_Template = {
    K.text: lambda concept: computeClassLabel(concept),
    K.name: 'Rectangle',
    K.corner_radius: 6,
    ...
    K.gradient_color: "Snow"}
```

The primary operation on a template is to *apply* it to some modeling object, typically a concept class or instance:

```
def apply_template(t, obj, time=None):
    # t.values are drawing-app values, or functions
    # obj: any object, passed into template functions
    # returns copy of t, F(obj) replaces functions F
    if isinstance(t, dict):
        return {k: apply_template(v, obj, time)
                for k, v in t.items()}
    if isinstance(t, list):
        return [apply_template(x, obj, time)
                for x in t]
    if callable(t):
        return t(obj) if arity(t)==1 else t(obj, time)
    return t
```

Animation templates have special case handling, since their functions take two parameters: the *instance* to be rendered, and the *time* at which to render its attributes.

Templates can also be *merged*. Figure 2 shows an instance of TableFunction as a circle in the same color as the TableFunction class, by merging an instance_template with a class_template.

7 SUMMARY

I have described PySTEMM as a tool, model library, and approach for building executable concept models for a variety of STEM subjects. The PySTEMM approach, using immutable objects and pure functions in Python, can apply to all STEM areas. It supports learning through pictures, narrative, animation, and graph plots, all generated from a single model definition, with minimal incidental complexity and code debugging issues. Such modeling, if given a more central role in K-12 STEM education, could make STEM learning much more deeply engaging.

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